

Maximum Estrada Index of Bicyclic Graphs*

Long Wang, Yi-Zheng Fan[†], Yi Wang

School of Mathematical Sciences, Anhui University, Hefei 230601, P. R. China

Abstract Let G be a simple graph of order n , let $\lambda_1(G), \lambda_2(G), \dots, \lambda_n(G)$ be the eigenvalues of the adjacency matrix of G . The Estrada index of G is defined as $EE(G) = \sum_{i=1}^n e^{\lambda_i(G)}$. In this paper we determine the unique graph with maximum Estrada index among bicyclic graphs with fixed order.

Keywords: Bicyclic graphs; Estrada index; eigenvalues

MR Subject Classifications: 05C50

1 Introduction

Let G be a simple graph of order n and let $A(G)$ be its adjacency matrix. The *eigenvalues* of G are referred to the eigenvalues of $A(G)$, denoted by $\lambda_1(G) \geq \lambda_2(G) \geq \dots \geq \lambda_n(G)$. The *Estrada index* $EE(G)$ of the graph G is defined as $EE(G) = \sum_{i=1}^n e^{\lambda_i(G)}$. The Estrada index was first introduced by Estrada [7] in 2000. It was found useful in biochemistry and complex networks, see [8, 9, 10, 11, 12]. Recently the Estrada index has been received a lot of attention in mathematics itself. Many bounds have been established for the Estrada index in [13, 15, 16, 14, 17]. Briefly, for a class \mathcal{S} of graphs, a graph $G \in \mathcal{S}$ is called *Estrada maximal* if $EE(G) \geq EE(H)$ for any $H \in \mathcal{S}$. The Estrada maximal trees subject to one or more graph parameters have been characterized; see [2, 4, 13, 16]. The unique Estrada maximal unicyclic graph was also determined in [6]. So, naturally the next problem is to characterize the Estrada maximal graph among all bicyclic graphs of fixed order. In this paper, we focus on this problem and determine the unique Estrada maximal graphs among all bicyclic graphs of fixed order.

A *bicyclic graph* $G = (V, E)$ is a connected simple graph which satisfies $|E| = |V| + 1$. There are two basic bicyclic graphs: ∞ -graph and θ -graph. More concisely, an ∞ -graph, denoted by $\infty(p, q, l)$, is obtained from two vertex-disjoint cycles C_p and C_q by connecting one vertex of C_p and one of C_q with a path P_l of length $l - 1$ (in the case of $l = 1$, identifying the above two vertices); and a θ -graph, denoted by $\theta(p, q, l)$, is a union of three internally disjoint paths $P_{p+1}, P_{q+1}, P_{l+1}$ of length p, q, l respectively with common end vertices, where $p, q, l \geq 1$ and at most one of them is 1. Observe that any bicyclic graph G is obtained from an ∞ -graph or a θ -graph G_0 (possibly) by attaching trees to some of its vertices. We call G_0 the *kernel* of G .

*Supported by National Natural Science Foundation of China (11071002), Program for New Century Excellent Talents in University, Key Project of Chinese Ministry of Education (210091), Specialized Research Fund for the Doctoral Program of Higher Education (20103401110002), Science and Technological Fund of Anhui Province for Outstanding Youth (10040606Y33), Scientific Research Fund for Fostering Distinguished Young Scholars of Anhui University (KJJQ1001), Academic Innovation Team of Anhui University Project (KJTD001B), Fund for Youth Scientific Research of Anhui University (KJQN1003).

[†]Corresponding author. E-mail addresses: fanyz@ahu.edu.cn (Y.-Z. Fan), wanglongxuzhou@126.com (L. Wang), wangy@ahu.edu.cn (Y. Wang)

2 Preliminaries and Lemmas

Let $M_k(G)$ be the k -th spectral moment of a graph G of order n , i.e., $M_k(G) = \sum_{i=1}^n \lambda_i^k(G)$. It is well known that $M_k(G)$ is equal to the number of closed walks of length k in G . The following result reveals the connection between the spectral moments and Estrada index:

$$EE(G) = \sum_{k=0}^{\infty} \frac{M_k(G)}{k!}.$$

For any vertices u, v and w (not necessary be distinct) in G , we denote by $M_k(G; u, v)$ the number of walks in G with length k from u to v , and by $M_k(G; u, v, [w])$ the number of walks in G with length k from u to v which go through w . Denote by $W_k(G; u, v)$ a walk of length k from u to v in G , and by $\mathcal{W}_k(G; u, v)$ the set of all such walks. Clearly $M_k(G; u, v) = |\mathcal{W}_k(G; u, v)|$.

Let G_1 and G_2 be two graphs with $u_1, v_1 \in V(G_1)$ and $u_2, v_2 \in V(G_2)$. We write $(G_1; u_1, v_1) \preceq (G_2; u_2, v_2)$ if $M_k(G_1; u_1, v_1) \leq M_k(G_2; u_2, v_2)$ for any positive integer k . If, in addition, $M_k(G_1; u_1, v_1) < M_k(G_2; u_2, v_2)$ for at least one positive integer k , then we write $(G_1; u_1, v_1) \prec (G_2; u_2, v_2)$. Surely $(G_1; u_1, v_1) = (G_2; u_2, v_2)$ implies $M_k(G_1; u_1, v_1) = M_k(G_2; u_2, v_2)$ for any positive integer k .

LEMMA 2.1 [3] *Let G be a graph containing two vertices u, v . Suppose that $w_i \in V(G)$ and $uw_i \notin E(G), vw_i \notin E(G)$ for $i = 1, 2, \dots, k$. Let $E_u = \{uw_i, i = 1, 2, \dots, k\}$ and $E_v = \{vw_i, i = 1, 2, \dots, k\}$. Let $G_u = G + E_u$ and $G_v = G + E_v$. If $(G; u, u) \prec (G; v, v)$ and $(G; u, w_i) \preceq (G; v, w_i)$ for $1 \leq i \leq k$, then $EE(G_u) < EE(G_v)$.*

The *coalescence* of two vertex-disjoint connected graphs G, H , denoted by $G(u) \circ H(w)$, where $u \in V(G)$ and $w \in V(H)$, is obtained by identifying the vertex u of G with the vertex w of H . A graph is called *nontrivial* if it contains at least two vertices.

LEMMA 2.2 [5] *Let G be a connected graph containing two vertices u, v , and let H be a nontrivial connected graph containing a vertex w . If $(G; u, u) \succ (G; v, v)$, then $EE(G(u) \circ H(w)) > EE(G(v) \circ H(w))$.*

LEMMA 2.3 [5] *Let H_1 be a nontrivial connected graph containing a vertex w , and let H_2 be a connected graph of order at least 3 containing an pendant edge uv , where v is a pendant vertex. Then $EE(H_1(w) \circ H_2(u)) > EE(H_1(w) \circ H_2(v))$.*

LEMMA 2.4 *Let H_1 be a connected graph containing two vertices u, v , and let H_2 be a connected graph disjoint to H_1 , which contains a vertex w . Let H'_2 be a copy of H_2 , containing the vertex w' corresponding to w of H_2 . Let $G = (H_1(u) \circ H_2(w))(v) \circ H'_2(w')$. If there exists an automorphism σ of H_1 such that it interchanges u and v , then $(G; u, u) = (G; v, v)$ and $(G; u, t) = (G; v, \sigma(t))$ for any vertex t distinct to u .*

Furthermore, if letting \bar{H}_1 be obtained from H_1 by adding some edges incident with v but not u , letting \bar{H}'_2 be obtained from H'_2 by adding some vertices or edges such that the resulting graph is connected, and letting \bar{G} be obtained from G by replacing H_1 with \bar{H}_1 or H'_2 with \bar{H}'_2 , then $(\bar{G}; u, u) \prec (\bar{G}; v, v)$ and $(\bar{G}; u, t) \prec (\bar{G}; v, \sigma(t))$ for any vertex t distinct to u .

Proof. Surely σ induces an automorphism of G , and also induces a 1-1 map from $\mathcal{W}_k(G; x, y)$ to $\mathcal{W}_k(G; \sigma(x), \sigma(y))$ for any x, y and k . The first assertion follows.

Now we prove the second assertion. Note that

$$M_k(\bar{G}; u, u) = M_k(\bar{G} - v; u, u) + M_k(\bar{G}; u, u, [v]), M_k(\bar{G}; v, v) = M_k(\bar{G} - u; v, v) + M_k(\bar{G}; v, v, [u]);$$

and

$$\begin{aligned}
M_k(\bar{G} - v; u, u) &= M_k((\bar{H}_1 - v)(u) \circ H_2(w); u, u) \\
&= M_k((H_1 - v)(u) \circ H_2(w); u, u) \\
&= M_k((H_1 - u)(v) \circ H'_2(w'); v, v),
\end{aligned}$$

where the last equality holds as σ induces an isomorphism between $(H_1 - v)(u) \circ H_2(w)$ and $(H_1 - u)(v) \circ H'_2(w')$ and interchanges u and v . However,

$$M_k(\bar{G} - u; v, v) = M_k((\bar{H}_1 - u)(v) \circ \bar{H}'_2(w'); v, v).$$

Since H_1 is a proper subgraph of \bar{H}_1 or H'_2 is a proper subgraph of \bar{H}'_2 , we have

$$M_k(\bar{G} - v; u, u) \leq M_k(\bar{G} - u; v, v)$$

with strict inequality for at least one k .

For each walk $W \in \mathcal{W}_k(\bar{G}; u, u, [v])$, write it as $W = W_1 W_2$, where W_1 is the longest subwalk of W from u to v , and W_2 is the remaining section from v to u . Define a map $f : \mathcal{W}_k(\bar{G}; u, u, [v]) \rightarrow \mathcal{W}_k(\bar{G}; v, v, [u])$ by $f(W) = W_2 W_1$. One can verify f is an injection, and hence $M_k(\bar{G}; u, u, [v]) \leq M_k(\bar{G}; v, v, [u])$. So we proved $(\bar{G}; u, u) \prec (\bar{G}; v, v)$. The proof of $(\bar{G}; u, t) \prec (\bar{G}; v, \sigma(t))$ can be argued in a similar way. \square

Denote by $N_G(v)$ the set of neighbors of a vertex v in a graph G , and by $d_G(v)$ the cardinality of the set $N_G(v)$.

COROLLARY 2.5 *Let G be a unicyclic graph obtained from a cycle C by attaching some trees on its vertices. Assume u, w are two adjacent vertices on the cycle C such that the tree attached at u is a star centered at v with one of its pendant vertices identified with u , and the tree attached at w is a star with its center identified with w ; see Fig. 2.1. If $d_G(w) \geq d_G(v) + 1$, then*

- (i) $(G; w, w) \succ (G; v, v)$;
- (ii) $(G; w, t) \succ (G; v, t)$ for any $t \notin (N_G(v) \cup N_G(w) \cup \{w\}) \setminus V(C)$.

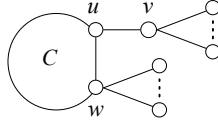


Fig. 2.1. An illustration of the graph G in Corollary 2.5

Proof. Let G' be the graph obtained from G by deleting the edge on the cycle incident to w except uw , and deleting $d_G(w) - d_G(v) - 1$ pendant vertices of w . Then there exists an automorphism of G' which interchanges v and w together with their pendant vertices, and preserves all other vertices. Now the assertion follows from the second result of Lemma 2.4. \square

COROLLARY 2.6 *Let G be obtained from $\theta(2, 2, l)$ by attaching some pendant edges at the vertices of its cycles. Let u, v, w, t be the vertices as shown in Fig. 2.2.*

- (i) *If $d_G(w) > 2$ and $d_G(t) = 2$, then $(G; w, w) \succ (G; t, t)$;*
- (ii) *If $d_G(u) > 3$, $d_G(v) = 3$ and $d_G(x) = 2$ for any $x \in V(G) \setminus \{u, v, w\}$, then $(G; u, u) \succ (G; v, v)$;*
- (iii) *If $d_G(u) > 3$, $d_G(v) = 3$ and $d_G(x) = 2$ for any $x \in V(G) \setminus \{u, v\}$, then $(G; u, u) \succ (G; w, w)$.*

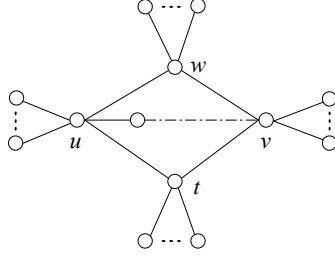


Fig. 2.2. An illustration of the graph G in Corollary 2.6

Proof. For the assertion (i), let G' be obtained from G by deleting the pendant vertices of w . Then there exists an automorphism σ of G' which interchanges w, t and preserves all other vertices. The assertion follows from Lemma 2.4. The assertions (ii),(iii) can be argued in a similar way by Lemma 2.4. ■

LEMMA 2.7 *Let $G = \theta(p, q, l)$ and let u, v be the two vertices of G with degree 3 respectively. Then $(G; u, u) = (G; v, v) \succ (G; w, w)$ for any vertex w distinct to u and v .*

Proof. Let $P_{p+1}, P_{q+1}, P_{l+1}$ be respectively the induced paths of G joining u and v . Define an automorphism σ of the graph G as follows: σ interchanges u and v , and for each vertex x of the path P_{p+1} (respectively, P_{q+1}, P_{l+1}), $\sigma(x)$ is also on P_{p+1} (respectively, P_{q+1}, P_{l+1}) such that the distance between x and u along this path is equal to that between $\sigma(x)$ and $v = \sigma(u)$. The automorphism σ naturally induces a map from $\mathcal{W}_k(G; s, t)$ to $\mathcal{W}_k(G; \sigma(s), \sigma(t))$, such that $\sigma(W_k(G; s, t)) = W_k(G; \sigma(s), \sigma(t))$ for any k and $s, t \in V(G)$, where each vertex x of $W_k(G; s, t)$ is mapped to $\sigma(x)$. In particular, σ is a 1-1 map from $\mathcal{W}_k(G; u, u)$ to $\mathcal{W}_k(G; v, v)$ for any k , and hence $(G; u, u) = (G; v, v)$.

To prove $(G; u, u) \succ (G; w, w)$ for any vertex w distinct to u and v , we only consider the case when w lies on the internal part of the path P_{l+1} . The other cases can be proved in a similar way. Denote C_{ij} the cycle made by P_{i+1} and P_{j+1} , where $i \neq j$, and i, j is one of p, q, l . One can easily see that $M_k(C_{ql}; u, u) = M_k(C_{ql}; w, w)$. Thus it suffices to consider the closed walks of length k from w to w that pass through at least one edge of P_{p+1} . Suppose that $W_k(G; w, w)$ is such a walk. We decompose the walk $W_k(G; w, w)$ into three parts W_1, W_2, W_3 in a unique way, where W_1 starts at w and goes along the path P_{l+1} as far as possible, whose terminal point must be u or v ; W_2 starts at the terminal point of W_1 , takes the first step and the last step on edges of C_{pq} , and $W - W_2$ contains no edges of C_{pq} , whose terminal point must be u or v ; $W_3 = W - W_1W_2$.

Now we construct a map g from $\mathcal{W}_k(G; w, w)$ to $\mathcal{W}_k(G; u, u)$ in the following way. If W_2 is a $u - u$ walk or $u - v$ walk, $g(W_1W_2W_3) = W_2W_3W_1$; if W_2 is a $v - u$ walk, $g(W_1W_2W_3) = W_3W_1W_2$; if W_2 is a $v - v$ walk, $g(W_1W_2W_3) = \sigma(W_3W_1W_2)$. By directly checking we find that g is an injection. Thus $M_k(G; u, u) \geq M_k(G; w, w)$ for any k . Obviously, $M_2(G; u, u) = 3 > 2 = M_2(G; w, w)$. This completes the proof. □

3 Main results

Denote by $\mathcal{G}_\infty(n; p, q)$ the set of all bicyclic graphs of order n which contains an ∞ -graph as a kernel with two cycles having length p, q respectively. Denote by $\mathcal{G}_\theta(n; p, q)$ the set of all bicyclic graphs of order n which contains $\theta(p', q', l')$ as kernel, where $p' \geq q' \geq l'$ and $p' + l' = p, q' + l' = q$. We first investigate some properties of Estrada maximal graphs in $\mathcal{G}_\infty(n; p, q)$ or $\mathcal{G}_\theta(n; p, q)$, and show that any Estrada maximal graph in $\mathcal{G}_\infty(n; p, q)$ will have a smaller Estrada index than some graph in $\mathcal{G}_\theta(n; p, q)$. Finally we determine the unique Estrada maximal graph among all bicyclic graphs of fixed order.

LEMMA 3.1 *If G is an Estrada maximal graph among all bicyclic graphs of order n , then G is obtained from its kernel by attaching some pendant edges.*

Proof. Assume to the contrary, there exists a pendant edge G not attached to its kernel. Then there is a cut edge uw of G such that $G - uw$ has two components G_1, G_2 , where G_1 contains the vertex u and the kernel of G , and G_2 is a nontrivial tree containing the vertex w . Removing G_2 at w and attaching it to u , by Lemma 2.3 we will arrive at a new bicyclic graph but with larger Estrada index, a contradiction. \square

THEOREM 3.2 *If G is an Estrada maximal graph in $\mathcal{G}_\infty(n; p, q)$, then G is obtained from $\infty(p, q, 1)$ by attaching some pendant edges.*

Proof. Suppose G is the Estrada maximal graph in $\mathcal{G}_\infty(n; p, q)$, and contains $\infty(p, q, l)$ as its kernel. By Lemma 3.1, G is obtained from $\infty(p, q, l)$ by attaching some pendant edges. We assert $l = 1$. Otherwise, let P_l ($l > 1$) be the path connecting C_p and C_q , and let $v_1 v_2$ be the starting edge of P_l , where $v_1 \in V(C_p)$. Write $G = G_1(v_1) \circ G_2(v_1)$, where G_1 contains C_p , and G_2 contains C_q and the vertex v_1 as a pendant vertex. Removing G_1 at v_1 and attaching it to v_2 , we will arrive at a graph $G' \in \mathcal{G}_\infty(n; p, q)$. However, by Lemma 2.3, $EE(G') > EE(G)$, a contradiction. \square

THEOREM 3.3 *If G is an Estrada maximal graph in $\mathcal{G}_\theta(n; p, q)$, then G is obtained from $\theta(p-1, q-1, 1)$ or $\theta(2, 2, 2)$ by attaching some pendant edges.*

Proof. Suppose G is an Estrada maximal graph in $\mathcal{G}_\theta(n; p, q)$, and contains $\theta(p', q', l')$ as its kernel, where $p' \geq q' \geq l'$ and $p' + l' = p, q' + l' = q$. By Lemma 3.1, G is obtained from $\theta(p', q', l')$ by attaching some pendant edges. If $l' = 1$, or $l' = 2$ and $p' = q' = 2$, the result follows. Now assume $l' \geq 2$ and $p' \geq 3$. Let u, v, w, t be the vertices of $\theta(p', q', l')$ as shown in the left graph of Fig. 3.1. Without loss of generality, assume $d_G(w) \geq d_G(v)$. Deleting the edge tv and adding a new edge tw , we will arrive at a new graph \bar{G} whose kernel is $\theta(p' - 1, q' - 1, l')$ as shown in the right graph in Fig. 3.1. Consider the unicyclic graph $G - tv$. By Lemma 2.5, $(G - tv; w, w) \succ (G - tv; v, v)$ and $(G - tv; w, t) \succ (G - tv; v, t)$. So, by Lemma 2.1, $EE(\bar{G}) > EE(G)$, a contradiction. \square

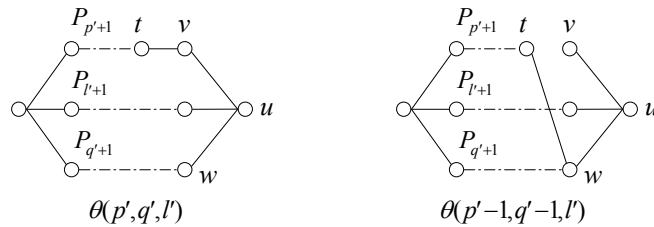


Fig. 3.1. An illustration of the proof of Theorem 3.3

LEMMA 3.4 *Let G be a bicyclic graph which is obtained from $\infty(p, q, 1)$ by attaching some pendant edges to its vertices. Then there exists a bicyclic graph \bar{G} whose kernel is $\theta(p-1, q-1, 1)$ such that $EE(\bar{G}) > EE(G)$.*

Proof. Let v, w, t be the vertices of $\infty(p, q, 1)$ as shown in Fig. 3.2, where $d_G(w) \geq d_G(v)$. Deleting the edge tv and adding a new edge tw , we will arrive at a new graph \bar{G} whose kernel is $\theta(p-1, q-1, 1)$ as shown in Fig. 3.2. Consider the unicyclic graph $G - tv$. By Lemma 2.5, $(G - tv; w, w) \succ (G - tv; v, v)$ and $(G - tv; w, t) \succ (G - tv; v, t)$. So, by Lemma 2.1, $EE(\bar{G}) > EE(G)$, a contradiction. \square

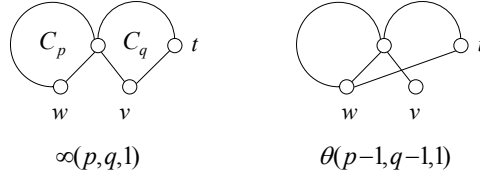


Fig. 3.2. An illustration of proof of Lemma 3.4

Denote by \mathbf{G}_1 the bicyclic graph of order n obtained from $\theta(2, 2, 1)$ by attaching $n - 4$ pendant edges to one of its vertices of degree 3, and by \mathbf{G}_2 the bicyclic graph of order n obtained from $\theta(2, 2, 2)$ by attaching $n - 5$ pendant edges to one of its vertices of degree 3.

LEMMA 3.5 *Let G be an Estrada maximal graph among all bicyclic graphs of order n . Then G is either \mathbf{G}_1 or \mathbf{G}_2 .*

Proof. By Theorem 3.2 and Lemma 3.4, G must contain a θ -graph as its kernel. By Lemma 3.3, G is obtained from $\theta(p, q, 1)$ or $\theta(2, 2, 2)$ by attaching some pendant edges. Assume G contains $\theta(p, q, 1)$ as its kernel, where $p \geq q$ and $p \geq 3$. Let v, w, t be the vertices of $\theta(p, q, 1)$ as shown in Fig. 3.3, where $d_G(w) \geq d_G(v)$. Deleting the edge tv and adding a new edge tw , we will arrive at a new graph \bar{G} whose kernel is $\theta(p-1, q-1, 2)$ as shown in Fig. 3.3. By a similar discussion to the proof of Lemma 3.4, we have $EE(\bar{G}) > EE(G)$, a contradiction. So G is obtained from $\theta(2, 2, 1)$ or $\theta(2, 2, 2)$ by attaching some pendant edges.

We next show all the pendant edges of G are attached at a unique vertex $\theta(2, 2, 1)$ or $\theta(2, 2, 2)$ with degree 3, and hence G is exactly \mathbf{G}_1 or \mathbf{G}_2 . We only prove the case of G having $\theta(2, 2, 2)$ as the kernel; the other case can be discussed in a similar way. Let $v_i, i = 1, 2, \dots, 5$, be the vertices of $\theta(2, 2, 2)$ as shown in the last graph in Fig. 3.3. Assume each v_i is attached to m_i pendant edges in the graph G , for $i = 1, 2, \dots, 5$, where $m_i \geq 0$ and $\sum_{i=1}^5 m_i = n - 5$.

Denote $G = G(m_1, m_2, m_3, m_4, m_5)$. If at least two of m_3, m_4, m_5 are nonzero, say $m_3 > 0, m_4 > 0$, by Corollary 2.6(i), $(G(m_1, m_2, m_3, 0, m_5; v_3, v_3)) \succ (G(m_1, m_2, m_3, 0, m_5; v_4, v_4))$, and by Lemma 2.2 removing all the pendant edges of $G(m_1, m_2, m_3, m_4, m_5)$ at v_4 and attaching them to v_3 , we will get a graph $G(m_1, m_2, m_3 + m_4, 0, m_5)$ with a larger Estrada index, a contradiction. So, at least two of m_3, m_4, m_5 are zero, say $m_4 = m_5 = 0$. Then $G = G(m_1, m_2, m_3, 0, 0)$.

If both m_1, m_2 are nonzero, by Corollary 2.6(ii), $(G(m_1, 0, m_3, 0, 0; v_1, v_1)) \succ (G(m_1, 0, m_3, 0, 0; v_2, v_2))$, and by Lemma 2.2 removing all the pendant edges of $G(m_1, m_2, m_3, 0, 0)$ at v_2 and attaching them to v_1 , we will arrive at graph $G(m_1 + m_2, 0, m_3, 0, 0)$ with a larger Estrada index, also a contradiction. So at least one of m_1, m_2 is zero, say $m_2 = 0$, i.e. $G = G(m_1, 0, m_3, 0, 0)$. By Lemmas 2.7 and 2.6, $(G(m_1, 0, 0, 0, 0; v_1, v_1)) \succ (G(m_1, 0, 0, 0, 0; v_3, v_3))$ whether or not $m_1 = 0$. If $m_3 > 0$, by a similar discussion we get $EE(G(m_1 + m_3, 0, 0, 0, 0)) > EE(G(m_1, 0, m_3, 0, 0))$, a contradiction. So $G = G(m_1, 0, 0, 0, 0)$, and the result follows. \square

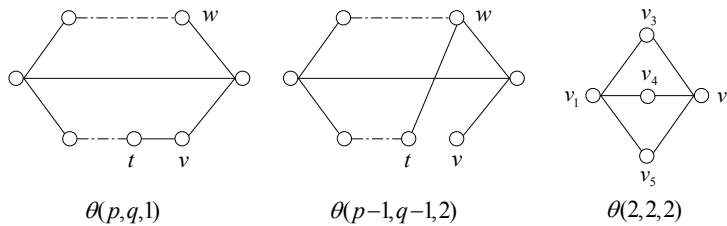


Fig. 3.3. An illustration of proof of Lemma 3.5

Finally we determine which is larger between $EE(\mathbf{G}_1)$ and $EE(\mathbf{G}_2)$. Denote by $\phi(G, x)$ the characteristic polynomial of the adjacency matrix of a graph G .

LEMMA 3.6 [1] *Let G be a graph containing a vertex v , and let $\mathcal{C}(v)$ be the set of cycles containing v . Then*

$$\phi(G, x) = x\phi(G - v, x) - \sum_{w \in N_G(v)} \phi(G - v - w, x) - 2 \sum_{Z \in \mathcal{C}(v)} \phi(G - V(Z), x).$$

PROPOSITION 3.7 $EE(\mathbf{G}_1) > EE(\mathbf{G}_2)$ for $n \geq 5$.

Proof. By Proposition 3.6, $\phi(\mathbf{G}_1, x) = x^{n-4}f(x)$, $\phi(\mathbf{G}_2, x) = x^{n-4}g(x)$, where

$$f(x) = x^4 - (n+1)x^2 - 4x + 2(n-4), g(x) = x^4 - (n+1)x^2 + 3(n-5).$$

By a direct calculation, $EE(\mathbf{G}_1) > EE(\mathbf{G}_2)$ when $5 \leq n \leq 22$. Now assume $n \geq 23$. Since $f(\sqrt{n-1}) = -6 - 4\sqrt{n-1} < 0$, $\lambda_1(\mathbf{G}_1) > \sqrt{n-1}$. On the other hand, as $g(x)$ is increasing for $x > \sqrt{\frac{n+1}{2}}$, $g\left(\sqrt{n-\frac{3}{2}}\right) = \frac{n}{2} - \frac{45}{4} > 0$ when $n \geq 23$, which implies $\lambda_1(\mathbf{G}_2) < \sqrt{n-\frac{3}{2}}$ when $n \geq 23$.

Let u, v be the vertices of \mathbf{G}_1 and \mathbf{G}_2 both with maximal degree, respectively. The graph $\mathbf{G}_1 - u$ has eigenvalues $\pm\sqrt{2}$ and 0 with multiplicity $n-3$, and the graph $\mathbf{G}_2 - v$ has eigenvalues $\pm\sqrt{3}$ and 0 with multiplicity $n-3$. By interlacing property of the eigenvalues of $A(\mathbf{G}_1 - u)$ and $A(\mathbf{G}_1)$ (or see [1]), $\lambda_i(\mathbf{G}_1) \geq \lambda_i(\mathbf{G}_1 - u)$ for $i = 2, 3, \dots, n-1$. So

$$EE(\mathbf{G}_1) = \sum_{i=1}^n e^{\lambda_i(\mathbf{G}_1)} > e^{\lambda_1(\mathbf{G}_1)} + \sum_{i=2}^{n-1} e^{\lambda_i(\mathbf{G}_1 - u)} > e^{\sqrt{n-1}} + (n-3) + e^{-\sqrt{2}}.$$

Similarly, by the fact $\lambda_i(\mathbf{G}_2) \leq \lambda_{i-1}(\mathbf{G}_2 - v)$ for $i = 2, 3, \dots, n$,

$$EE(\mathbf{G}_2) \leq e^{\lambda_1(\mathbf{G}_2)} + \sum_{i=2}^n e^{\lambda_i(\mathbf{G}_2 - v)} < e^{\sqrt{n-\frac{3}{2}}} + e^{\sqrt{3}} + (n-3) + e^{-\sqrt{3}}.$$

Noting that $e^{\sqrt{n-1}} > e^{\sqrt{n-\frac{3}{2}}} + e^{\sqrt{3}}$ for $n \geq 23$, so we get the result. \square

By Lemma 3.5 and Proposition 3.7, we get the main result of this paper.

THEOREM 3.8 *Let G be a bicyclic graph of order n . Then $EE(G) \leq EE(\mathbf{G}_1)$, with equality if and only if $G = \mathbf{G}_1$.*

References

- [1] D. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs-Theory and Application*, Academic Press, New York, 1980.
- [2] H. Deng, A proof of a conjecture on the Estrada index, *MATCH Commun. Math. Comput. Chem.*, 62 (2009) 599-606.
- [3] Z. Du, Z. Liu, On the Estrada and Laplacian Estrada indices of graphs, *Linear Algebra Appl.*, 435 (2011) 2065-2076.
- [4] Z. Du, B. Zhou, The Estrada index of trees, *Linear Algebra Appl.*, 435 (2011) 2462-2467.
- [5] Z. Du, B. Zhou, On the Estrada index of graphs with given number of cut vertices, *Electron. J. Linear Algebra*, 22 (2011) 586-592.
- [6] Z. Du, B. Zhou, The Estrada index of unicyclic graphs, *Linear Algebra Appl.*, 436 (2012) 3149-3159.
- [7] E. Estrada, Characterization of 3D molecular structure, *Chem. Phys. Lett.*, 319 (2000) 713-718.

- [8] E. Estrada, Characterization of the folding degree of proteins, *Bioinformatics*, 18 (2002) 697-704.
- [9] E. Estrada, Characterization of the amino acid contribution to the folding degree of proteins, *Proteins*, 54 (2004) 727-737.
- [10] E. Estrada, J. A. Rodríguez-Valázquez, Subgraph centrality in complex networks, *Phys. Rev. E*, 71 (056103) (2005) 1-9.
- [11] E. Estrada, J. A. Rodríguez-Valázquez, Spectral measures of bipartivity in complex networks, *Phys. Rev. E*, 72 (046105) (2005) 1-6.
- [12] E. Estrada, J. A. Rodríguez-Valázquez, M. Randić, Atomic branching in molecules, *Int. J. Quantum Chem.*, 106 (2006) 823-832.
- [13] A. Ilíc, D. Stevanović, The Estrada index of chemical trees, *J. Math. Chem.*, 47 (2010) 305-314.
- [14] W. Li, A. Chang, On the trees with maximum nullity, *MATCH Commun. Math. Comput. Chem.*, 2006, 56(3) 501-508.
- [15] J. A. de la Peña, I. Gutman, J. Rada, Estimating the Estrada index, *Linear Algebra Appl.*, 427 (2007) 70-76.
- [16] J. Zhang, B. Zhou, J. Li, On Estrada index of trees, *Linear Algebra Appl.*, 434 (2011) 215-223.
- [17] B. Zhou, On Estrada index, *MATCH Commun. Math. Comput. Chem.*, 60 (2008) 485-492.
- [18] B. Zhou, N. Trinajstić, Estrada index of bipartite graphs, *Int. J. Chem. Model.*, 1 (2008) 387-394.